Distribution-Free PCE Surrogate Models for Efficient Structural Reliability Analysis

HyeongUk Lim and Lance Manuel
Mechanics, Uncertainty, and Simulation in Engineering
Civil, Architectural and Environmental Engineering

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Outline

Structural Reliability Methods

- Sampling
  - Monte Carlo Simulation $\rightarrow$ accurate, but time-consuming
  - Latin Hypercube, Importance Sampling, Subset Simulation
- Geometric approximation
  - FORM and SORM
- Surrogate model
  - Polynomial Chaos Expansion (PCE) $\rightarrow$ our focus
  - Kriging
  - Artificial Neural Network (ANN)
- PDF derivation:
  - Kernel density estimation
  - Maximum entropy distribution
  - Method of moments

Surrogate Limit State Functions

- Accurate prediction of probability of failure is essential for structural safety.
- Limit state functions can involve the use of expensive computational models.
- Can benefit from “surrogate” functions that serve as approximations for the “truth” limit state functions.

$$\underbrace{g(\boldsymbol{x})}_{\text{truth}} \approx \underbrace{\hat{g}(\boldsymbol{x})}_{\text{surrogate}}$$

hours per a run
vs.
seconds per 10^6 runs

Probability of Failure

Probability of failure using the truth limit state function:

$$P_\mathrm{f} = P[g \leq 0] \approx \frac{1}{N} \sum_{i=1}^{N} I[g(\boldsymbol{x}^{(i)}) \leq 0]$$

Probability of failure using a surrogate limit state function:

$$\hat{P}_\mathrm{f} = P[\hat{g} \leq 0] \approx \frac{1}{N} \sum_{i=1}^{N} I[\hat{g}(\boldsymbol{x}^{(i)}) \leq 0]$$

Appropriate development of $\hat{g}$ is needed to yield:

$$P_\mathrm{f} \approx \hat{P}_\mathrm{f}$$

Polynomial Chaos Expansion (PCE)

A limit state function can be represented by using PCE:

$$g(\boldsymbol{X}) \overset{\text{PCE}}{\approx} \hat{g}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}^d} c_{\boldsymbol{\alpha}} \cdot \Psi_{\boldsymbol{\alpha}}(T(\boldsymbol{X}))$$

α: multi-indicial coefficients
c: coefficients to be estimated
$\Psi(.)$: orthogonal polynomials
$T(.)$: iso-probabilistic transformation

- Any function of inputs can be represented by orthogonal basis functions defined in auxiliary input-space.

Formal Approach of PCE: Askey Scheme

- Orthogonal polynomial family is defined for the selected independent variables for best convergence ratio.

  ex) Hermite polynomials for Gaussian variables

- For complex random variables or dependent random variables, an iso-probabilistic transformation is needed.

  ex) Multi-modal random variables
  Complex dependency structures

- But non-linearity of the transformation may limit PCE.

Non-linearity in T

$$\underset{\text{truth model of } \boldsymbol{X}}{g(\boldsymbol{X})} \overset{T}{=} \underset{\text{truth model of } \boldsymbol{Q}}{g(\boldsymbol{Q})} \approx \underset{\text{PCE of } \boldsymbol{Q}}{\hat{g}(\boldsymbol{Q})}$$

- $T : \boldsymbol{X} \to \boldsymbol{Q}$ may be nonlinear.
- $g(\boldsymbol{Q})$ becomes complicated.
- PCE aims to fit $g(\boldsymbol{Q})$, not $g(\boldsymbol{X})$

Limitations of Traditional PCE

Cases that limit traditional PCE use:

- non-standard distributions (outside the Askey variables)
- dependence pattern among the input variables

For such problems, one must go beyond Askey scheme polynomial families.

Arbitrary Polynomial Chaos Expansion (APCE)

Recall: a limit state function represented by using PCE:

$$g(\boldsymbol{X}) \overset{\text{PCE}}{\approx} \hat{g}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d} c_{\boldsymbol{\alpha}} \cdot \Psi_{\boldsymbol{\alpha}}(T(\boldsymbol{X}))$$

α: multi-indicial coefficients
c: coefficients to be estimated
$\Psi(.)$: orthogonal polynomials
$T(.)$: iso-probabilistic transformation

We can use Gram-Schmidt orthogonalization to establish basis polynomials instead of using Askey type polynomials that involve iso-probabilistic transformations.

$$g(\boldsymbol{X}) \overset{APCE}{\approx} \hat{g}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathbb{N}^d} c_{\boldsymbol{\alpha}} \cdot P_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

Univariate Basis Polynomial Functions

A univariate polynomial basis function of order, p, generated by Gram-Schmidt orthogonalization:

$$P_X^{(p)}(x) = \det \begin{bmatrix} m_0 & m_1 & \dots & m_p \\ m_1 & m_2 & \dots & m_{p+1} \\ \vdots & \vdots & \vdots & \vdots \\ m_{p-1} & m_p & \dots & m_{2p-1} \\ 1 & x & \dots & x^p \end{bmatrix}$$

m_k is the kth raw moment of X.

$P_X^{(p)}(x)$ can be tensorized to define a multivariate orthogonal polynomial function. But non-product type probability measures in the dependent variables cannot be accounted for.

Multivariate Basis Polynomial Functions

Define a multivariate polynomial basis function as:

$$P_{\alpha}(\boldsymbol{x}) = \frac{1}{\Delta_{n-1,d}} \cdot \det \begin{bmatrix} \boldsymbol{m}_{\{0\}+\{0\}} & \cdots & \boldsymbol{m}_{\{0\}+\{n-1\}} & \boldsymbol{m}_{\alpha,0} \\ \vdots & \ddots & \vdots & \vdots \\ \boldsymbol{m}_{\{n-1\}+\{0\}} & \cdots & \boldsymbol{m}_{\{n-1\}+\{n-1\}} & \boldsymbol{m}_{\alpha,n-1} \\ & & & \\ (\boldsymbol{x}^0)^{\mathsf{T}} & \cdots & (\boldsymbol{x}^{n-1})^{\mathsf{T}} & x^{\alpha} \end{bmatrix}$$

$$\Delta_{n-1,d} = \det \begin{bmatrix} \boldsymbol{m}_{\{0\}+\{0\}} & \cdots & \boldsymbol{m}_{\{0\}+\{n-1\}} \\ \vdots & \ddots & \vdots \\ \boldsymbol{m}_{\{n-1\}+\{0\}} & \cdots & \boldsymbol{m}_{\{n-1\}+\{n-1\}} \end{bmatrix}$$

Multivariate Basis Polynomial Functions (Cont'd)

Define a monomial, $x^{\boldsymbol{\alpha}}$:

$$x^{\boldsymbol{\alpha}} = x_1^{\alpha_1} \cdots x_d^{\alpha_d}$$

x^n denotes a column vector, $\mathrm{x}^n \equiv [\forall x^{\boldsymbol{\alpha}}]^\mathsf{T}$, such that $|\boldsymbol{\alpha}| = n$.

A moment matrix, $\boldsymbol{m}_{\{i\}+\{j\}}$:

$$\boldsymbol{m}_{\{i\}+\{j\}} \equiv \mathbb{E}[\mathrm{x}^i(\mathrm{x}^j)^T]$$

A moment vector, $\boldsymbol{m}_{\boldsymbol{\alpha},i}$:

$$\boldsymbol{m}_{\boldsymbol{\alpha},i} \equiv \mathbb{E}[x^{\boldsymbol{\alpha}}\mathrm{x}^i]$$

PCE Coefficient Estimation

The PCE coefficients can be estimated by linear regression:

$$\boldsymbol{c} = \arg \min_{\boldsymbol{c} \in \mathbb{R}^{N_p}} \sum_{k=1}^{N_s} \left[g(\boldsymbol{x}^{(k)}) - \sum_{|\boldsymbol{\alpha}| \leq p} c_{\boldsymbol{\alpha}} P_{\boldsymbol{\alpha}}(\boldsymbol{x}^{(k)}) \right]^2$$

N_p: number of PCE coefficients
N_s: number of simulations in the truth system

Metric for Model Evaluation

The root-mean-square error (RMSE) to assess global accuracy of models:

$$\mathrm{RMSE} = \sqrt{\frac{1}{N_T}\sum_{k=1}^{N_T}\left(g^{(k)}(\boldsymbol{x}) - \hat{g}^{(k)}(\boldsymbol{x})\right)^2}$$

N_T: total number of evaluations

The maximum absolute error (MAE) to assess local accuracy of models:

$$\mathrm{MAE} = \max_{k=1,\cdots,N_T} |g^{(k)}(\boldsymbol{x}) - \hat{g}^{(k)}(\boldsymbol{x})|$$

Example 1: Noisy Limit State Function

$$g_{\mathbf{X}}(\mathbf{x}) = x_1 + 2x_2 + 2x_3 + x_4 - 5x_5 - 5x_6 + 0.001\sum_{i=1}^{6}\sin(100x_i)$$

Variable	Distribution	Mean	COV
X_1	Lognormal	120	0.10
X_2	Lognormal	120	0.10
X_3	Lognormal	120	0.10
X_4	Lognormal	120	0.10
X_5	Lognormal	50	0.30
X_6	Lognormal	40	0.30

	MCS	APCE	HPCE
		$p = 1$	$p = 4$
σ_{P_f}	3.28×10^{-4}	3.28×10^{-4}	3.28×10^{-4}
μ_{P_f}	1.23×10^{-2}	1.23×10^{-2}	1.23×10^{-2}
COV	2.68×10^{-2}	2.68×10^{-2}	2.68×10^{-2}
RMSE		2.10×10^{-3}	1.12×10^{-1}
MAE		9.10×10^{-3}	7.13×10^{0}
N_s		21	630

Example 2: Quadratic Function

$$\begin{aligned} g_{\boldsymbol{X}}(\boldsymbol{x}) \\ &= 1.1 - 0.00115x_1x_2 + 0.00157x_2^2 \\ &+ 0.00117x_1^2 + 0.0135x_2x_3 - 0.0705x_2 \\ &- 0.00534x_1 - 0.0149x_1x_3 - 0.0611x_2x_4 \\ &+ 0.0717x_1x_4 - 0.226x_3 + 0.0333x_3^2 \\ &- 0.558x_3x_4 + 0.998x_4 - 1.339x_4^2 \end{aligned}$$

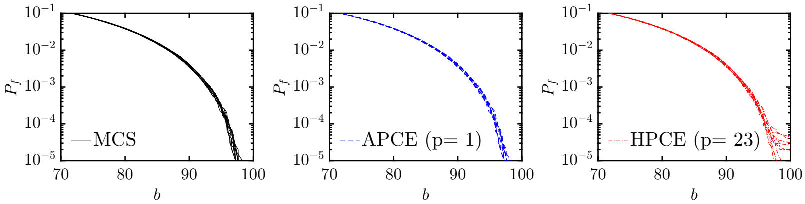
Variable	Distribution	Mean	COV
X_1	Type II Extreme	10	0.50
X_2	Normal	25	0.20
X_3	Normal	0.8	0.25
X_4	Lognormal	0.0625	1.00

	MCS	APCE	HPCE
		$p = 2$	$p = 10$
σ_{P_f}	6.89×10^{-4}	6.89×10^{-4}	6.96×10^{-4}
μ_{P_f}	5.57×10^{-2}	5.57×10^{-2}	5.57×10^{-2}
COV	1.24×10^{-2}	1.24×10^{-2}	1.25×10^{-2}
RMSE		6.90×10^{-16}	1.40×10^{-1}
MAE		1.31×10^{-14}	3.88×10^{1}
N_s		45	3003

Example 3: Correlated Non-Normal Variables

$$g_{\boldsymbol{X}}(\boldsymbol{x}) = b - (x_1 - x_2)$$
$$\rho_{X_1,X_2} = 0.5$$

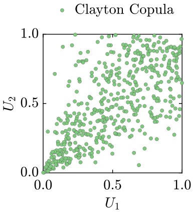
Variable	Distribution	Mean	COV
X_1	Uniform	50	0.58
X_2	Exponential	12.5	1

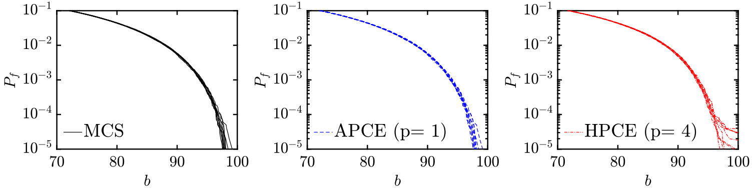


- MCS is based on 1×10^6 truth model evaluations.
- APCE requires only 9 evaluations of the truth model.
- Traditional PCE using Hermite polynomials (HPCE) requires 900 evaluations, and is still not satisfactory in the region where $P_f < 10^{-4}$.

Example 3 with a Non-Gaussian Dependence Structure

A non-Gaussian dependence structure (Clayton copula with $\theta = 2$) is investigated.





- APCE again shows good agreement in the prediction of the failure probabilities.
- HPCE clearly suffers in displaying good convergence to the truth model.

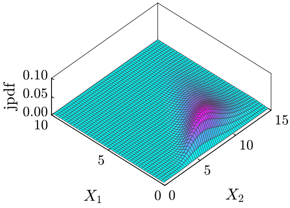
Example 4: Dependence Structure Defined by Rosenblatt Transformation

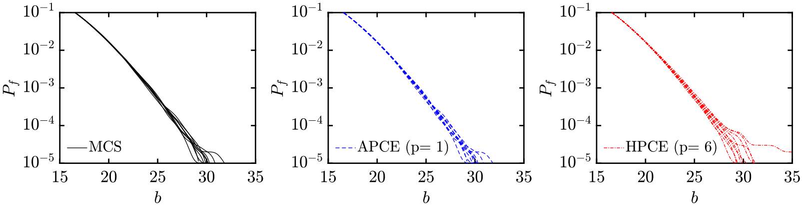
$$g_{\mathbf{X}}(\mathbf{x}) = b - (x_1 + x_2)$$

X_1 : lognormal and Weibull combined

X_2 : lognormal conditional on X_1

jpdf : $f_{X_1,X_2}(x_1, x_2) = f_{X_1}(x_1) f_{X_2|X_1}(x_2|x_1)$





- A dependence structure defined by a Rosenblatt transformation is investigated.
- APCE is able to deal with the complex dependence structure.

Example 5: Multimodal Random Variables

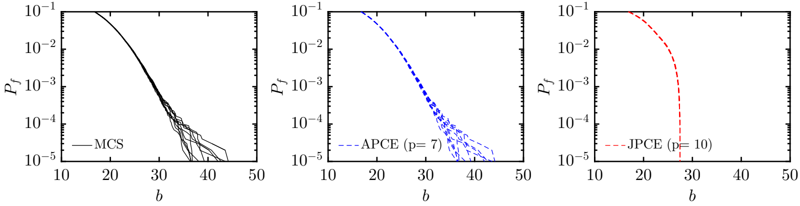
The Ishigami function with modification in the support for the variables:

$$g_{\mathbf{X}}(\mathbf{x}) = b - (\sin x_1 + 7\sin^2 x_2 + 0.1 x_3^4 \sin x_1)$$

X_i follows a mixture distribution with a pdf:

$$f(x) = \sum_{i=1}^{3} w_i \phi_i(x)$$

w_i: 1/3, ϕ_i: Gaussian pdfs with: $(\mu, \sigma) =$ $(2.0, 0.1)$, $(2.5, 0.5)$, $(3.5, 0.2)$



- APCE predicts accurate results even when X_i exhibits multimodal characteristics.
- JPCE (Jacobi polynomials) clearly fails.

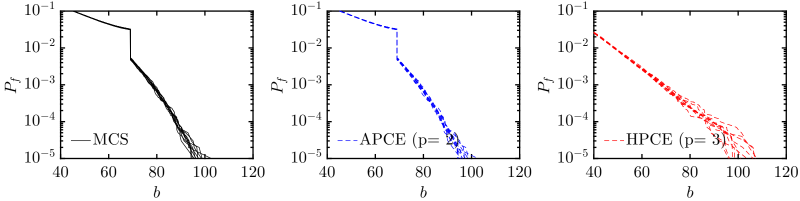
Example 6: Mixed Discrete-Continuous Support

A quadratic performance function is given as:

$$g_{\mathbf{X}}(\mathbf{x}) = b - (15 + 4x_1x_2 + 4x_1x_3 + 4x_2x_3 + 3x_1 + 3x_2 + 3x_3 - x_1^2 - x_2^2 - x_3^2)$$

X_i follows a mixture distribution with a pdf:

$$f_X(x) = 0.7\left(\frac{1}{\sqrt{2\pi}}\exp(-\frac{x^2}{2})\right) + 0.3\delta(x - 2.0)$$



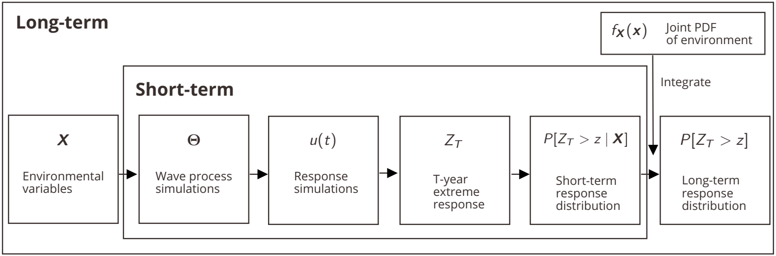
- APCE yields accurate results, even with the mixed discrete-continuous variables.
- HPCE clearly does not.

Example 7: Time-Domain Simulation-Based Extremes for an Offshore System - Implicit Performance Function

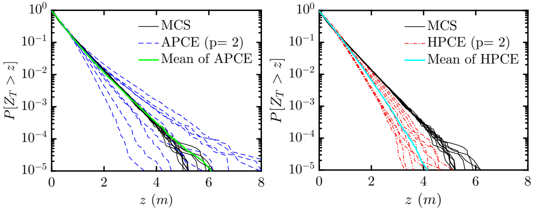
A generic offshore system performance function:

$$g = z - Z_T(\boldsymbol{X})$$

z: threshold value
Z_T: T-year long-term extreme response



Example 7: Time-Domain Simulation-Based Extremes for an Offshore System - Implicit Performance Function (Cont'd)



- To account for the the different short- and long-term uncertainty variables, we use ten surrogates, each with a total of 600 samples.
- APCE with $p = 2$ yields comparable long-term response estimates, with significantly less effort compared with MCS ($600 : 10^6$).

Conclusions

- A distribution-free PCE framework for efficient structural reliability analysis is proposed.
- Gram-Schmidt orthogonalization utilizes joint raw moments of random variables to construct multivariate polynomial basis functions.
- The proposed method is validated using benchmark problems as well as an offshore design problem.
- Results suggest that APCE is more versatile and accurate compared to traditional PCE (Askey scheme).

TEXAS

The University of Texas at Austin